Characterizing entanglement with geometric entanglement witnesses

Philipp Krammer*

Faculty of Physics, University of Vienna,
Boltzmanngasse 5, A-1090 Vienna, Austria

We show how to detect entangled, bound entangled, and separable bipartite quantum states of arbitrary dimension and mixedness using geometric entanglement witnesses. These witnesses are constructed using properties of the Hilbert-Schmidt geometry and can be shifted along parameterized lines. The involved conditions are simplified using Bloch decompositions of operators and states. As an example we determine the three different types of states for a family of two-qutrit states that is part of the "magic simplex", i.e. the set of Bell-state mixtures of arbitrary dimension.

I. INTRODUCTION

Entanglement is a fascinating curiosity of quantum physics that distinguishes it considerably from classical concepts [1]. On the one hand it implicates surprising philosophical aspects such as the incompatibility of local realistic theories with quantum physics [2, 3], on the other hand it can be successfully implied in quantum information and quantum communication tasks to improve quantum protocols with respect to classical ones (for an overview see, e.g., Refs [4, 5, 6]).

It is still an open mathematical problem to determine whether a quantum state is entangled or not, there is no operational procedure for an arbitrary state, although there are many useful criteria that allow a detection of entanglement in many cases [7, 8, 9]. For pure states and lower dimensional bipartite systems (e.g., two qubits) the problem is solved, since there exist applicable necessary and sufficient conditions for separability (i.e. non-entanglement) [10]. Additionally, entangled states can be classified according to their *distillability*: A distillable state can be "distilled" to a (nearly) maximally entangled state via statistical local operations and classical communication (SLOCC). States that are not distillable are called *bound entangled*, whereas distillable states are called *free entangled* [9, 11, 12, 13]. Examples of bound entangled states and construction procedures can be found in Refs. [14, 15, 16, 17, 18].

In this article we want to present a method to classify entanglement with entanglement witnesses, which provide a well-established tool to detect entanglement. Our approach is based on two concepts: We construct witnesses in a geometrically intuitive way and use Bloch decompositions of operators and states to simplify the mathematical application. We show how to use geometric entanglement witnesses to detect more entangled states than the PPT criterion and how to identify separable states by using optimal entanglement witnesses. This is attained by shifting the witnesses along parameterized lines of states. Two main methods are explained in detail: the *outside-in shift* and the *inside-out shift*. The *outside-in shift*

*Electronic address: philipp.krammer[at]univie.ac.at

is used for detecting more (bound) entangled states, whereas with the *inside-out shift* we construct the shape of the set of separable states.

The paper is organized as follows: In Sec. II we give an overview of the mathematical basics of entanglement theory that will be used throughout this article. We present a formulation of the entanglement witness criterion in terms of Bloch decompositions in Sec. III and explain a geometric method to construct entanglement witnesses in Sec. IV, where we also introduce the two shift methods. The results are applied to a family of states that are part of a special simplex (called "magic simplex") in the Hilbert-Schmidt space of two qutrits in Sec. V, where illustrative geometric pictures are obtained identifying regions of entangled, bound entangled, and separable states.

II. BASIC CONCEPTS OF ENTANGLEMENT THEORY

We consider a bipartite Hilbert-Schmidt space $\mathcal{A} := \mathcal{A}_A \otimes \mathcal{A}_B$ on a discrete finite dimensional Hilbert space $\mathcal{H} := \mathcal{H}_A \otimes \mathcal{H}_B$ of dimension $d_A \times d_B$, $D := d_A d_B$. Vector states $|\psi\rangle$ are elements of $\mathcal{H}$ whereas density operators (called "density matrices" or just "states") are elements of $\mathcal{A}$, a Hilbert space of operators on $\mathcal{H}$, with a scalar product

$$\langle A, B\rangle = \mathrm{Tr} A^\dagger B, \quad \text{with } A,\, B \in \mathcal{A}\,. \tag{1}$$

States $\rho \in \mathcal{A}$ are defined by the properties

$$\rho^\dagger = \rho,\ \mathrm{Tr}\rho = 1,\ \rho \geq 0\,, \tag{2}$$

i. e. they are Hermitian, have trace one, and are positive semidefinite, i.e. have nonnegative eigenvalues. For the sake of simplicity we will often drop the term "semidefinite" in the text and write "positive" only, meaning positive semidefinite. All states ρ satisfy the inequality $\mathrm{Tr}\rho^2 \leq 1$, and are classified as pure states ($\mathrm{Tr}\rho^2 = 1$) or mixed states ($\mathrm{Tr}\rho^2 < 1$).

The Hilbert-Schmidt distance of two states ρ_1 and ρ_2 is given by

$$d(\rho_1, \rho_2) := \|\rho_1 - \rho_2\| := \langle \rho_1 - \rho_2, \rho_1 - \rho_2\rangle^{1/2}\,. \tag{3}$$

Density operators can be represented as a matrix using an orthonormal basis of $\mathcal{H}$. The standard basis representation is

$$\rho_{ij,kl} := \langle ij|\rho|kl\rangle \tag{4}$$

where $|ij\rangle := |i\rangle \otimes |j\rangle$ and $\{|ij\rangle\}$ is the standard product basis of a $d_A \times d_B$ dimensional system.

A state ρ is called *entangled* if it cannot be written as a convex combination of product states [19],

$$\rho \neq \sigma = \sum_i p_i \rho_A^i \otimes \rho_B^i\,, \tag{5}$$

where ρ_A^i and ρ_B^i are states of the two subsystems, usually called "Alice" and "Bob" following the convention of quantum communication. States σ (5) are called *separable*, they are not entangled and contain classical correlations only. There is still no operational method (i.e., no "recipe") to decide for a given bipartite state of arbitrary dimension wether it it can be written as the convex combination (5) or not. This problem is known as the separability problem. However, there exist several criteria which help to find the entanglement properties of states in special cases, for an overview see, e.g., Refs. [7, 9, 20]

A criterion that is necessary and sufficient, but not operational, is the entanglement witness criterion (EWC) [10, 21, 22, 23, 24]. It says that a state ρ is entangled if and only if it can be "witnessed" by some Hermitian operator A, for which

$$\langle \rho, A \rangle \; = \; \mathrm{Tr}\, \rho A \; < \; 0 \,, \tag{6}$$

$$\langle \sigma, A \rangle = \mathrm{Tr}\, \sigma A \; \geq \; 0 \qquad \forall\, \sigma \in \mathcal{S} \,, \tag{7}$$

where $\mathcal{S}$ denotes the convex and compact set of all separable states, and A is called an *entanglement witness*. We call inequality (6) "entanglement condition" and inequality (7) "separability condition". If there exists a separable state $\tilde{\sigma}$ for which $\mathrm{Tr}\tilde{\sigma}A = 0$, then A is called an *optimal* entanglement witness. It is closest to the set of separable states and thus detects more entangled states than non-optimal witnesses.

The EWC is a consequence of the Hahn-Banach theorem of functional analysis. It geometrically corresponds to the fact that an element of a Banach space can always be separated by a hyperplane from a convex and compact subset that does not contain the element (see, e.g., Ref. [25] and Refs. [7, 24] for illustrations). Although it is intuitive and simple, the EWC is not easy to implement given an arbitrary state ρ, since in general it is difficult to find a suitable witness that satisfies Eq. (7), and even more difficult to state that there does not exist any witness for this state, which would imply separability. Nevertheless the criterion plays an important role in the theoretical understanding of entanglement, and has the advantage that a witness A corresponds to a physical observable that can be implemented in experiments. It therefore allows a detection of entanglement without performing a full tomography of the state [26, 27, 28, 29, 30].

An operational criterion that is a necessary condition for separability is the positive partial transpose (PPT) criterion [31]. It simply says that a separable state σ stays positive under partial transposition,

$$\sigma^{\Gamma} := (\mathbb{1} \otimes T)\sigma \geq 0 \,, \tag{8}$$

where the partial transpose is a transposition T with respect to Bob's system only, $\rho^{\Gamma}_{ij,kl} := \rho_{il,kj}$. As a proof of Eq. (8) one just has to recognize that if we apply the partial transposition to a separable state (5) the transposition is performed on ρ^i_B only, which does not change the positivity of the state, and thus the whole separable state stays positive. Therefore, if a state ρ violates the criterion, i.e. it is no longer positive under partial transposition, it has to be an entangled state. We call a state that is positive under partial transposition PPT, and a state that is not NPT. For dimensions 2×2 and 2×3 it can be shown that the criterion is necessary and sufficient [10], i.e. any entangled state has to be NPT. In higher dimensions, however, there exist entangled states that are PPT, it can be proven that such states are bound entangled. Note that the reverse is not necessarily true, it is still an open question if all NPT states are free entangled, although there are strong implications that NPT bound entangled states exist [32, 33].

In order to find PPT entangled states, one has to employ criteria that are not equal to or weaker than the PPT criterion. In principle the EWC is strongest since it detects the entanglement of all entangled states, but it is more cumbersome to apply.

Another useful criterion is the realignment criterion (or cross norm criterion) [34, 35, 36, 37], which again is a necessary condition for separability. It states that for any separable state the sum of the singular values s_i of a *realigned* density matrix σ_R has to be smaller than or equal to one,

$$\sum_i s_i = \mathrm{Tr}\sqrt{\sigma_R^{\dagger}\sigma_R} \leq 1 \,, \tag{9}$$

where $(\rho_{ij,kl})_R := \rho_{ik,jl}$. The realignment criterion is neither weaker nor stronger than the PPT criterion, meaning that it detects some entangled states that the PPT criterion does not, and vice versa. Thus an application of both criteria is easy to perform and allows a detection of many entangled states, both free and bound entangled, but they do not constitute a necessary and sufficient criterion together, since there exist PPT entangled states that are not detected by the realignment criterion [37].

III. BLOCH DECOMPOSITIONS AND ENTANGLEMENT WITNESSES

Bloch decompositions are a convenient way to handle calculations in high dimensional systems, since the usage of large matrices can be avoided (for an overview see [38] and references therein). There also exist computable separability criteria based on Bloch decompositions of states [39, 40].

Let us consider the Hilbert-Schmidt space for a one-particle state first, for example the space of Alice's subsystem $\mathcal{A}_A$ on $\mathcal{H}_A$ of dimension $d_A := d$ (all considerations are equivalent for Bob). Since the Hilbert-Schmidt space $\mathcal{A}_A$ is a vector space of operators, one can decompose any element of $\mathcal{A}_A$ into a linear combination of operators that form an orthogonal basis of the Hilbert-Schmidt space. Let us identify such a basis of d^2 operators with $\{\mathbb{1}, A_i\}$, $i = 1, \ldots, d^2 - 1$. The operators A_i are traceless, $\mathrm{Tr} A_i = 0$ and satisfy the orthogonality condition

$$\mathrm{Tr} A_i A_j = N_A \delta_{ij}, \quad N_A \in \mathbb{R}\,. \tag{10}$$

A one-particle qudit state can then be decomposed into the operator basis as (for example a state ρ_A for Alice's subsystem of dimension d)

$$\rho_A = \frac{1}{d}\left(\mathbb{1} + \sqrt{\frac{d(d-1)}{N_A}} \sum_{i=1}^{d^2-1} n_i A_i\right), \quad n_i \in \mathbb{C}\,, \tag{11}$$

where $|\vec{n}|^2 = \sum_i n_i^* n_i \leq 1$. The coefficient vector $\vec{n}$ is called *Bloch vector*, it uniquely characterizes the state. The constant $\sqrt{d(d-1)/N_A}$ results from the inequality $\mathrm{Tr}\rho^2 \leq 1$. The state is pure if and only if $|\vec{n}|^2 = 1$. In general not all arbitrary vectors $\vec{n}$ are Bloch vectors, i.e. they do not necessarily imply $\rho \geq 0$, see Remark 1.

A bipartite product state $\sigma_p := \rho_A \otimes \rho_B$ on $\mathcal{H}$ of dimension $d_A \times d_B$ can be written as (where Bob's orthogonal basis is $\{\mathbb{1}, B_j\}$)

$$\sigma_p = \frac{1}{d^2}\Big(\mathbb{1}_{\mathrm{d_A}} \otimes \mathbb{1}_{\mathrm{d_B}} + \sum_{i=0}^{d_A^2-1} f_A\, n_i\, A_i \otimes \mathbb{1}_{\mathrm{d_B}} + \sum_{j=0}^{d_B^2-1} f_B\, m_j\, \mathbb{1}_{\mathrm{d_A}} \otimes B_j + \sum_{i,j} f_A f_B\, n_i m_j A_i \otimes B_j\Big)\,,$$

$$n_{nm}, m_{lk} \in \mathbb{C}\,,\ |\vec{n}| \leq 1\,,\ |\vec{m}| \leq 1\,, \quad f_A := \sqrt{\frac{d_A(d_A-1)}{N_A}},\ f_B := \sqrt{\frac{d_B(d_B-1)}{N_B}}\,, \tag{12}$$

where the state is pure if and only if $|\vec{n}| = |\vec{m}| = 1$.

Any operator $O \in \mathcal{A}$ can be decomposed as

$$O = e\, \mathbb{1}_{\mathrm{d_A}} \otimes \mathbb{1}_{\mathrm{d_B}} + \sum_{i=0}^{d_A^2-1} a_i\, A_i \otimes \mathbb{1}_{\mathrm{d_B}} + \sum_{j=0}^{d_B^2-1} b_j\, \mathbb{1}_{\mathrm{d_A}} \otimes B_j + \sum_{i,j} c_{ij} A_i \otimes B_j\,,$$

$$e, a_i, b_i, c_{ij} \in \mathbb{C}\,. \tag{13}$$

For a given operator O and same dimensions of the subsystems $d_A = d_B =: d$, one can always find an orthogonal basis in which the coefficient matrix $C^{cor} = (c_{ij})$, called *correlation coefficient matrix*, is diagonal: Given an operator decomposition (13), we have to perform a singular value decomposition of C,

$$S = U C^{cor} V^{\dagger} \,, \tag{14}$$

where U and V are unitary matrices with entries u_{ij} and v_{ij} and S is the resulting diagonal matrix with the d^2 diagonal real positive singular values s_i of C^{cor} as diagonal entries. The new basis operators D_i^A and D_i^B are then given by a linear combination of the old operators,

$$D_i^A = \sum_j u_{ij}^* A_j , \quad D_i^B = \sum_j v_{ij} B_j \,, \tag{15}$$

which satisfy the same orthogonality condition, $\mathrm{Tr} D_i^A D_j^A = N_A \delta_{ij}$ (and equivalently for D_i^B). So we can rewrite Eq. (13) as

$$O = e\, \mathbb{1}_{\mathrm{d}} \otimes \mathbb{1}_{\mathrm{d}} + \sum_{i=0}^{d^2-1} r_i\, D_i^A \otimes \mathbb{1}_{\mathrm{d}} + \sum_{j=0}^{d^2-1} t_j\, \mathbb{1}_{\mathrm{d}} \otimes D_j^B + \sum_{i,j} s_i D_i^A \otimes D_i^B \,, \tag{16}$$

where $r_i = \sum_j a_j u_{ij}, \ t_j = \sum_k b_k v_{jk}^*$ and $s_i = \sum_{j,l} u_{ij} c_{jl} v_{il}^*$. We call the decomposed operator that is written in the optimized way of Eq. (16) "singular value optimized" (SVO). Of course a product state can then also be decomposed in terms of the new basis,

$$\sigma_p = \frac{1}{d^2}\Big(\mathbb{1}_{\mathrm{d}} \otimes \mathbb{1}_{\mathrm{d}} + \sum_{i=0}^{d^2-1} f_A\, \bar{n}_i\, D_i^A \otimes \mathbb{1}_{\mathrm{d}} + \sum_{j=0}^{d^2-1} f_B\, \bar{m}_j\, \mathbb{1}_{\mathrm{d}} \otimes D_j^B + \sum_{i,j} f_A f_B\, \bar{n}_i \bar{m}_j D_i^A \otimes D_j^B \Big) ,$$
$$\bar{n}_i, \bar{m}_j \in \mathbb{C} \,, \quad \big|\vec{\bar{n}}\big| \le 1 \,, \quad \big|\vec{\bar{m}}\big| \le 1 \,. \tag{17}$$

For our purposes we want to reformulate the separability condition (7) of the EWC:

Corollary 1. *An operator $C \in \mathcal{A}$ satisfies $\mathrm{Tr}\sigma C \ge 0 \ \forall \sigma \in S$ if and only if $\mathrm{Tr}\sigma_p C \ge 0$ for all pure product states $\sigma_p := \rho_A \otimes \rho_B$.*

Proof. If we have $\mathrm{Tr}\sigma C \ge 0 \ \forall \sigma \in S$ then of course also $\mathrm{Tr}\sigma_p C \ge 0$ since the pure pruduct states σ_p are separable states as well. A separable state (5) can be written as a convex combination of *pure* product states, $\sigma = \sum_i p_i \sigma_p^i$, because mixed states ρ_A and ρ_B are convex combinations of pure states. Thus if $\mathrm{Tr}\sigma_p C \ge 0$, it follows that $\mathrm{Tr}\sigma C = \mathrm{Tr} \sum_i p_i \sigma_p^i C = \sum_i p_i \mathrm{Tr}\sigma_p^i C \ge 0$ since $p_i \ge 0$. □

At first sight Corollary 1 may appear redundant, but it bears the advantage that in order to check if a given operator satisfies the separability condition (7), we do not have to check all separable states but consider pure product states only, which implies a decrease in effort. Purity of the states is not essential, but is more convenient in parameterizations.

For an arbitrary operator basis we use the Bloch decomposition (13) to write an Hermitian operator $C \in \mathcal{A}$ as

$$C = \delta \left(\mu \mathbb{1}_{\mathrm{d_A}} \otimes \mathbb{1}_{\mathrm{d_B}} + \sum_{i=0}^{d_A^2-1} \tilde{a}_i\, A_i \otimes \mathbb{1}_{\mathrm{d_B}} + \sum_{j=0}^{d_B^2-1} \tilde{b}_j\, \mathbb{1}_{\mathrm{d_A}} \otimes B_j + \sum_{i,j} \tilde{c}_{ij} A_i \otimes B_j \right) ,$$
$$\mu := \sqrt{(d_A-1)(d_B-1)}, \ \delta \in \mathbb{R}^+ \,. \tag{18}$$

Note that we are only interested in Hermitian operators C with positive values of δ. If δ happens to be negative in the first place we switch to the operator with an additional overall minus sign. For $d_A = d_B = d$ we use Eq. (16) to obtain the SVO form

$$C = \delta\left((d-1)\mathbb{1}_{\mathrm{d}} \otimes \mathbb{1}_{\mathrm{d}} + \sum_{i=0}^{d^2-1} \tilde{r}_i\, D_i^A \otimes \mathbb{1}_{\mathrm{d}} + \sum_{j=0}^{d^2-1} \tilde{t}_j\, \mathbb{1}_{\mathrm{d}} \otimes D_j^B + \sum_i \tilde{s}_i D_i^A \otimes D_i^B\right), \tag{19}$$

and get for the expectation value with product states σ_p from Eqs. (12) and (18) (we use $\sigma_p^\dagger$ in order to conveniently utilize the orthogonality condition (10))

$$\mathrm{Tr}\sigma_p^\dagger C = \delta\mu\left(1 + \sqrt{\frac{d_B}{N_B(d_B-1)}}\sum_i \tilde{a}_i n_i^* + \sqrt{\frac{d_A}{N_A(d_A-1)}}\sum_j \tilde{b}_j m_j^* + \sum_{i,j} \tilde{c}_{ij} n_i^* m_j^*\right), \tag{20}$$

which simplifies for $d_A = d_B = d$ to (using Eqs. (17) and (19))

$$\mathrm{Tr}\sigma_p^\dagger C = \delta(d-1)\left(1 + \sqrt{\frac{d}{N_B(d-1)}}\sum_i \tilde{r}_i \bar{n}_i^* + \sqrt{\frac{d}{N_A(d-1)}}\sum_j \tilde{t}_j \bar{m}_j^* + \sum_i \tilde{s}_i \bar{n}_i^* \bar{m}_i^*\right). \tag{21}$$

Using the above expressions for the expectation values we obtain a condition for $\mathrm{Tr}C\sigma_p \geq 0$ in Corollary 1 in terms of Bloch decompositions:

Corollary 2. *Given a decomposition* (18) *of an operator C into an arbitrary operator basis, the expectation value for any product state* (12) *is positive or vanishes,* $\mathrm{Tr}C\sigma_p \geq 0$*, if and only if*

$$S := \sqrt{\frac{d_B}{N_B(d_B-1)}}\sum_i \tilde{a}_i n_i^* + \sqrt{\frac{d_A}{N_A(d_A-1)}}\sum_j \tilde{b}_j m_j^* + \sum_{i,j} \tilde{c}_{ij} n_i^* m_j^* \geq -1 \tag{22}$$

for all Bloch vectors $\vec{n}$, $\vec{m}$. For equal dimensions of the subsystems, $d_A = d_B = d$, the condition (22) *can be simplified to*

$$S = \sqrt{\frac{d}{N_B(d-1)}}\sum_i \tilde{r}_i \bar{n}_i^* + \sqrt{\frac{d}{N_A(d-1)}}\sum_j \tilde{t}_j \bar{m}_j^* + \sum_i \tilde{s}_i \bar{n}_i^* \bar{m}_i^* \geq -1\,, \tag{23}$$

where we used the SVO form (19) *of C.*

Proof. The proof is evident from the expressions for the expectation values in Eqs. (20) and (21). □

Remark 1. Consider the case when there also exists at least one state ρ for which $\mathrm{Tr}C\rho < 0$. Then C is an entanglement witness if $S \geq -1$. Note that by stating "Bloch vector" we mean vectors $\vec{n}$ that correspond to states (i.e. $\rho_A \geq 0$ in Eq. (11)). For arbitrary dimensions d of the Hilbert space an arbitrary vector $\vec{n} \in \mathbb{C}^{d^2-1}$ for which ρ has real eigenvalues does not always implicate $\rho \geq 0$, this is only true for $d = 2$, where the familiar matrix basis out of the Pauli matrices or rotations thereof is used.

Remark 2. It directly follows from Corollaries 1 and 2 that C is an optimal entanglement witness if and only if there exists a state ρ such that $\mathrm{Tr}C\rho < 0$ and Bloch vectors $\vec{n}, \vec{m}$ such that $S = -1$.

Remark 3. For operators C (18) with vanishing coefficients $\tilde{a}_i$, $\tilde{b}_i$, condition (22) reduces to

$$\sum_{i,j} \tilde{c}_{ij} n_i^* m_j^* \geq -1 \tag{24}$$

and for $d_A = d_B$ condition (23) reduces to

$$\sum_{i} \tilde{s}_i \bar{n}_i^* \bar{m}_i^* \geq -1\,. \tag{25}$$

This is for example the case if we consider geometric operators (see Sec. IV) constructed of states that are *locally maximally mixed*, which means their reduced density matrices are the maximally mixed states $(1/d_A)\mathbb{1}$ and $(1/d_B)\mathbb{1}$.

Lemma 1. *For operators C (18) on a Hilbert space $\mathcal{H}$ of equal dimensional subsystems, $d_A = d_B$, with vanishing coefficients $\tilde{a}_i$, $\tilde{b}_i$, the expectation value for product states is greater or equal to zero, $\mathrm{Tr}\sigma_p \geq 0$, if the singular values $\tilde{s}_i$ of the correlation coefficient matrix $\tilde{c}_{ij}$ are smaller or equal to one, $\tilde{s}_i \leq 1$.*

Proof. With vanishing coefficients $\tilde{a}_i$, $\tilde{b}_i$, the term S in Eq. (22) reduces to $S = \sum_{i,j} \tilde{c}_{ij} n_i m_j$. For $d_A = d_B$ we can write the operator in SVO form, which gives $S = \sum_i \tilde{s}_i \bar{n}_i^* \bar{m}_i^*$. With the condition $s_i \leq 1$ we get

$$|S| = \left| \sum_i \tilde{s}_i \bar{n}_i^* \bar{m}_i^* \right| \leq \sum_i \tilde{s}_i |\bar{n}_i^*||\bar{m}_i^*| \leq \sum_i |\bar{n}_i^*||\bar{m}_i^*| \leq 1 \tag{26}$$

and thus $S \geq -1$. □

Remark 4. Note that Lemma 1 gives only a sufficient condition for satisfying the inequality $\mathrm{Tr}\sigma_p \geq 0$. It is necessary for dimensions 2×2 only, since in this case any vectors $\vec{n}_i$ and $\vec{m}_i$ (12) correspond to states, see Remark 1, and with at least one singular value $s_i \geq 1$ one can easily construct Bloch vectors such that $S < -1$. For higher dimensions it is possible that some $s_i > 1$, and still there exists no Bloch vectors $\vec{n}_i$ and $\vec{m}_i$ (that provide $\rho \geq 0$) such that $S < -1$.

IV. GEOMETRIC ENTANGLEMENT WITNESSES

Definition 1. A *geometric operator* $G \in \mathcal{A}$ is defined as

$$G := \rho_1 - \rho_2 - \langle \rho_1, \rho_1 - \rho_2 \rangle \mathbb{1}_D\,, \tag{27}$$

where ρ_1 and ρ_2 are arbitrary states in $\mathcal{A}$ and $\rho_1 \neq \rho_2$.

The definition originates from the construction of entanglement witnesses in Refs. [23, 39], with the difference that in our definition the geometric operator (27) does not yet have to be an entanglement witness. The construction (27) provides $\mathrm{Tr}\rho_1 G = 0$ and $\mathrm{Tr}\rho_2 G < 0$,

$$\begin{aligned}\mathrm{Tr}\rho_1 G &= \langle \rho_1, G\rangle = \langle \rho_1 - \rho_1, \rho_1 - \rho_2\rangle = 0\,,\\ \mathrm{Tr}\rho_2 G &= \langle \rho_2, G\rangle = \langle \rho_2 - \rho_1, \rho_1 - \rho_2\rangle = -\|\rho_1 - \rho_2\|^2 < 0\,.\end{aligned} \tag{28}$$

It corresponds to a hyperplane in the Hilbert-Schmidt space $\mathcal{A}$ that divides the whole state space into states ρ_n for which $\mathrm{Tr}\rho_n G < 0$ and states ρ_p for which $\mathrm{Tr}\rho_p G \geq 0$, see Ref [24]. The hyperplane is orthogonal to $\rho_1 - \rho_2$ since for all states ρ_G on the plane, i.e. that satisfy $\mathrm{Tr}\rho_G G = 0$, the operator $\rho_1 - \rho_2$ is orthogonal to $\rho_G - \rho_1$ because $\mathrm{Tr}\rho_G G = \langle \rho_G - \rho_1, \rho_1 - \rho_2\rangle = 0$.

Definition 2. A *geometric entanglement witness (GEW)* A_G is a geometric operator that satisfies $Tr\sigma_p A_G \geq 0$ for all pure product states σ_p.

Due to its construction, a geometric entanglement witness (see also Refs. [23, 24, 39, 41, 42, 43] has to witness at least the entanglement of ρ_2. For arbitrary states ρ_2 it is easy to construct geometric operators G (Definition 1) that ensure $\mathrm{Tr}\rho_2 G < 0$, but difficult to confirm that also $\mathrm{Tr}\sigma_p G \geq 0$ for all pure product states, which would yield $G = A_G$. Nevertheless, due to their simple geometric construction, geometric operators provide useful tools to characterize entanglement, as we will see in the further sections. Other methods to construct and optimize entanglement witnesses are given in Refs. [44, 45, 46, 47, 48].

To detect entanglement it is sufficient to consider geometric entanglement witnesses only:

Lemma 2. *Any entangled state is witnessed by a geometric entanglement witness.*

Proof. If ρ is entangled, then there exists a so-called *nearest separable state* σ_0, i.e. the separable state for which the Hilbert-Schmidt distance (3) from ρ to the set of separable states $\mathcal{S}$ is minimal, because $\mathcal{S}$ is convex and compact. The corresponding geometric operator $\sigma_0 - \rho - \langle \sigma_0, \sigma_0 - \rho\rangle \mathbb{1}_D$ is an entanglement witness, since the corresponding hyperplane includes σ_0, is orthogonal to $\sigma_0 - \rho$ and is therefore tangent to $\mathcal{S}$. For more details on nearest separable states see Refs. [23, 24, 49]. □

Geometric entanglement witnesses bear the advantage that they can be “shifted” along lines of parameterized states.

Proposition 1 (Shift method)**.** *If a geometric operator*

$$G_\lambda = \rho_\lambda - \rho - \langle \rho_\lambda, \rho_\lambda - \rho\rangle \mathbb{1}_{\mathrm{D}} \tag{29}$$

with a parameterized family of states

$$\rho_\lambda := \lambda\rho + (1-\lambda)\tilde{\rho}, \quad 0 \leq \lambda < 1,\ \ \rho, \tilde{\rho} \in \mathcal{A} \tag{30}$$

is an entanglement witness in a parameter region $\lambda \in [\lambda_i, 1)$*, i.e. if it satisfies* $\mathrm{Tr}\sigma_P G_\lambda \geq 0$ *for all pure product states* σ_P*, then* ρ_λ *is entangled for* $\lambda \in (\lambda_i, 1]$*.*

Proof. We consider states ρ_λ with $\lambda_i < \lambda \leq 1$ and the geometric entanglement witness $A_{\lambda_i} = \rho_{\lambda_i} - \rho - \langle \rho_{\lambda_i}, \rho_{\lambda_i} - \rho\rangle \mathbb{1}_{\mathrm{D}}$. The expectation value in ρ_λ is

$$\begin{aligned}\mathrm{Tr}\rho_\lambda A_{\lambda_i} &= \langle \rho_\lambda, A_{\lambda_i}\rangle = \langle \rho_\lambda - \rho_{\lambda_i}, \rho_{\lambda_i} - \rho\rangle\\ &= (\lambda_i - \lambda)(1-\lambda_i)\langle \rho - \tilde{\rho}, \rho - \tilde{\rho}\rangle = (\lambda_i - \lambda)(1-\lambda_i)\|\rho - \tilde{\rho}\|^2 < 0\,,\end{aligned} \tag{31}$$

hence the states ρ_λ with $\lambda_i < \lambda \leq 1$ are entangled. □

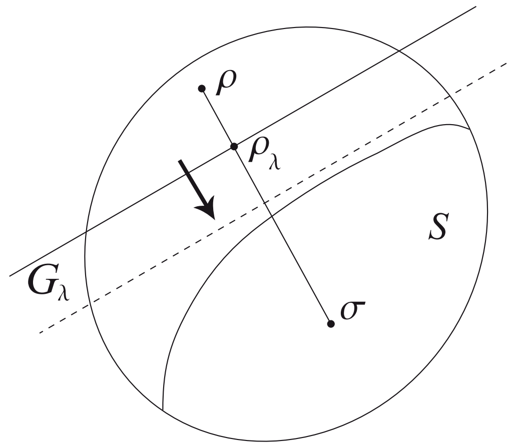

FIG. 1: Outside-in shift method. On the line between the entangled state ρ and the separable state σ one can detect more entangled states, e.g. bound entangled states, by shifting the geometric entanglement witness.

An effective way to use the shift method of Proposition 1 is to identify $\tilde{\rho}$ in Eq. (30) with a separable state, and ρ with a state which is known to be entangled. There are two cases where this is of particular interest:

1. (*Outside-in shift.*) Starting from the entangled state ρ, we can detect further entangled states along the line in direction to the separable state. By proofing that G_λ is an entanglement witness for a parameter region $\lambda_i \leq \lambda < 1$ (the case $\lambda = 1$ can be included with a suitable normalization of G_λ), one can infer that all states ρ_λ within this region are entangled. A reasonable choice for the separable state is the maximally mixed state $(1/D)\mathbb{1}$. In this way one can detect bound entangled states, for example if we choose a PPT entangled "starting state" ρ, then we are likely to find more bound entangled states along the parameterized line ρ_λ. The outside-in shift is illustrated in Fig. 1. See Refs. [42, 43] for application examples. In Ref. [50] a similar approach with parameterized lines between PPT entangled states and the maximally mixed state is used to identify families of bound entangled states in the context of robustness of entanglement.

2. (*Inside-out shift.*) Another application of the shift method is the step-by-step construction of the convex set of separable states. Here one has to use optimal GEWs that correspond to hyperplanes tangent to the set of separable states. Let us assume we are given a specific convex subset of states for which we want to determine the entanglement properties and that some separable states are known. From these we can constuct a *kernel polytope* of separable states, i.e. the convex hull of the known separable states. Then we assign geometric operators to hyperplanes tangent to the kernel polytope. For example, an operator corresponding to a plane that includes the line between two separable states can be constructed in the following way: Given two separable states σ_1 and σ_2, the convex line between them is $\sigma_\mu = \mu\sigma_1 + (1-\mu)\sigma_2$. Now we choose an entangled state ω, that of course lies outside the kernel polytope, such that there exists a μ_i with $\tilde{\sigma} = \sigma_{\mu_i}$ for which we have the orthogonality condition $\langle \sigma_1 - \sigma_2, \omega - \tilde{\sigma}\rangle = 0$. The geometric operator is then given by

$$G = \tilde{\sigma} - \omega - \langle \tilde{\sigma}, \tilde{\sigma} - \omega \rangle \mathbb{1}_{\mathrm{D}} \tag{32}$$

and a shift operator G_λ between $\tilde{\sigma}$ and ω according to Eqs. (29) and (30). The construction of operators that correspond to boundary planes of the kernel polygon identified by more than two separable states is done similarily, using more orthogonality conditions and the convex hull between three states.

Once we assigned geometric operators to the boundary of the kernel polytope, we utilize Proposition 1 to "shift" the operators outside and survey the minimum of S in Eq. (22) or (23). At one point of the parameterized line (30) we obtain $S = -1$; the geometric operators become optimal geometric entanglement witnesses. In this way we can assemble the shape of the set of separable states for the considered set of states and distinguish it from the set of entangled states. It may likely be that we have an idea of the shape of the set of separable states that we got from applying necessary separability criteria. Then we can use the inside-out shift to verify or falsify that shape: The inside-out shifted geometric operators should correspond to optimal GEWs when they become tangent to the estimated shape. In this way we get vertices of a new polytope, whose boundary planes are shifted again. Thus we either verify the estimated shape of separable states, or, if a shifted plane is an optimal GEW before it is tangent to the shape, it is an enclosure of all separable states and also entangled ones. We require finite steps of this method if the estimated shape is a polygon, and (in principle) infinite steps if it is not a polygon, i.e. if it has a curved surface.

If we have no idea of a possible shape of the set of separable states, or if our estimation turned out to be wrong, we can use the inside-out shift to obtain at least a tight enclosure polytope. It is a polytope that encloses all separable states but might also contain some entangled states, it can be obtained by applying the shift to more than one kernel polytope. Both situations are sketched in Fig. 2.

The difficult part of Proposition 1 is to prove that G_λ is an entanglement witness, in particular the verification of the separability condition (7). To accomplish this we can efficiently use the previous corollaries and lemmas, which will be demonstrated by the example of the next section.

V. ENTANGLEMENT PROPERTIES OF A FAMILY OF TWO-QUTRIT STATES

An interesting set of states is the *magic simplex* of two-qudit states (dimension $d \times d$) [51, 52, 53]. It is the set of all states that are mixtures of Bell states P_{nm},

$$\mathcal{W} := \left\{ \sum_{n,m=0}^{d-1} q_{nm} P_{nm} \mid q_{nm} \geq 0, \sum_{n,m} q_{nm} = 1 \right\}, \tag{33}$$

where the d^2 operators (the *Bell states*)

$$P_{nm} := (U_{nm} \otimes \mathbb{1}) |\phi_d^+\rangle\langle\phi_d^+| (U_{nm}^\dagger \otimes \mathbb{1}) \tag{34}$$

form an orthogonal basis of the $d \times d$ dimensional Hilbert space and the vector state $|\phi_d^+\rangle$ denotes the maximally entangled state

$$|\phi_d^+\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |j\rangle \otimes |j\rangle \,. \tag{35}$$

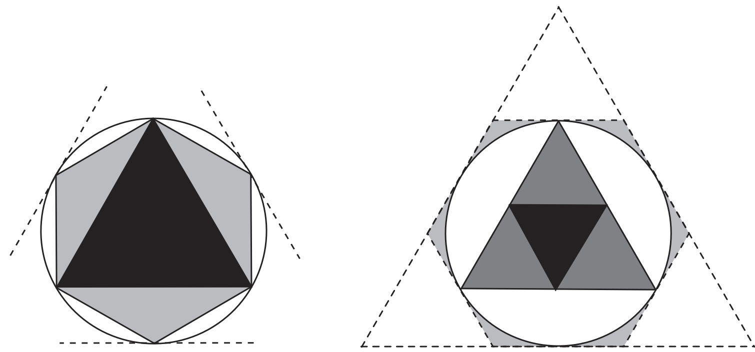

FIG. 2: Left: Sketch of the inside-out shift with an estimate of the shape of separable states, which in this case coincides with the true set of separable states, pictured by the circle. We start with a kernel polytope (black triangle) and shift the boundary planes outside until they become optimal GEWs, which are tangents to the circle (dashed lines). In this way we can draw a new polytope (hexagon, grey). In the next steps (not illustrated) the boundaries of the new polytope are shifted and we gain a new polytope, and so on. In this way we reconstruct the circle shape.
Right: Sketch of the inside-out shift where we do not rely on an estimate of the shape of separable states. The true set of separable states is again pictured by a circle. Here we get a first enclosure polytope (biggest triangle with dashed lines), by shifting the boundaries of a first kernel polytope outside (dark grey triangle). A tighter enclosure polytope (hexagon with dashed lines) is obtained by shifting the boundaries of a second kernel polytope (small black triangle) outside. The light grey areas mark states inside the enclosure polytope that are not separable and thus account for the deviation of the enclosure polytope from the true set of separable states.

The unitary operatos U_{nm} are the Weyl operators

$$U_{nm} = \sum_{k=0}^{d-1} e^{\frac{2\pi i}{d}\,kn}\, |k\rangle\langle (k+m) \,\mathrm{mod}\, d| \,, \tag{36}$$

which have been introduced in classical theories of discrete phase space and appear in quantum information theory in the context of quantum teleportation [54]. In the teleportation protocol the Bell state basis (34) is the higher dimensional generalization of the two-qubit basis and the Weyl operators U_{nm} are the analogue of the Pauli operators, they correspond to the operators Bob has to apply in order to obtain the teleported state. The reduced density operators of states that are elements of the magic simplex are maximally mixed, but not all two-qudit states with maximally mixed reduced density operators are elements of the magic simplex, apart from dimension 2×2, where all locally maximally mixed states are included in the tetrahedron of all Bell state mixtures [53]. Furthermore the magic simplex has a high symmetry in the phase space of the coefficients nm, for a detailed discussion see Refs. [51, 52].

The Weyl operators (36) form an orthogonal operator basis,

$$\mathrm{Tr}\, U_{nm}^{\dagger} U_{lj} = d\, \delta_{nl}\, \delta_{mj} \tag{37}$$

and hence can be used for Bloch decompositions. The Bell states P_{nm} (34) can be expressed

with Weyl operators as (where the indices have to be taken mod d)

$$P_{nk} = \frac{1}{d^2} \sum_{m,l=0}^{d-1} e^{\frac{2\pi i}{d}(kl-nm)}\, U_{lm} \otimes U_{-lm} = \frac{1}{d^2} \sum_{l,m=0}^{d-1} c_{lm}\, U_{lm} \otimes U_{-lm}\,. \tag{38}$$

Obviously the Bloch vectors corresponding to the Bell states have a diagonal but in general complex coefficient matrix (c_{ij}), where i counts the different combinations of lm and j those of kn, and $c_{ii} := c_{lm}$. The singular values of the coefficient matrix are $s_i = |c_{ii}| = |c_{lm}|$.

Note that a construction of the type (34) can be done with any unitary operators that form a matrix basis of the Hilbert-Schmidt space, obtaining other bases of orthogonal maximally entangled states.

A subset of the magic simplex of two-qutrit states (dimension 3×3) that reveals interesting entanglement characteristics is the three-parameter family [42, 43]

$$\rho_{\alpha,\beta,\gamma} := \frac{1-\alpha-\beta-\gamma}{9}\mathbb{1} + \alpha P_{00} + \frac{\beta}{2}\left(P_{10}+P_{20}\right) + \frac{\gamma}{3}\left(P_{01}+P_{11}+P_{21}\right)\,, \tag{39}$$

where the parameters are constrained by the positivity requirement $\rho_{\alpha,\beta,\gamma} \geq 0$,

$$\begin{aligned} &\alpha \leq \frac{7}{2}\beta + 1 - \gamma\,, \quad && \alpha \leq -\beta + 1 - \gamma\,, \\ &\alpha \leq -\beta + 1 + 2\gamma\,, \quad && \alpha \geq \frac{\beta}{8} - \frac{1}{8} + \frac{1}{8}\gamma\,. \end{aligned} \tag{40}$$

The family of states (39) contains a one-parameter family of states that have three entanglement properties; they can be separable, PPT entangled and NPT entangled. We call them Horodecki states ρ_b [16],

$$\rho_b = \frac{2}{7}\left|\phi_+^3\right\rangle\left\langle\phi_+^3\right| + \frac{b}{7}\sigma_+ + \frac{5-b}{7}\sigma_-\,, \qquad 0 \leq b \leq 5\,, \tag{41}$$

and, according to our parametrization,

$$\rho_b := \rho_{\alpha,\beta,\gamma} \qquad \text{with} \quad \alpha = \frac{6-b}{21},\ \beta = -\frac{2b}{21},\ \gamma = \frac{5-2b}{7}\,. \tag{42}$$

Using the PPT criterion we find regions of PPT and NPT Horodecki states: They are NPT for $0 \leq b < 1$, PPT for $1 \leq b \leq 4$ and again NPT for $4 < b \leq 5$. In Ref. [16] it is shown that the states are separable for $2 \leq b \leq 3$ and bound entangled for $3 < b \leq 4$.

Now let us apply the PPT criterion (8) and the realignment criterion (9) to our three-parameter family (39). The PPT criterion provides the following parameter constraints for PPT states $\rho_{\alpha,\beta,\gamma}$:

$$\begin{aligned} \alpha &\leq -\beta - \frac{1}{2} + \frac{1}{2}\gamma\,, \\ \alpha &\leq \frac{1}{16}\left(-2 + 11\beta + 3\sqrt{\Delta}\right)\,, \quad \alpha \geq \frac{1}{16}\left(-2 + 11\beta - 3\sqrt{\Delta}\right)\,, \end{aligned} \tag{43}$$

where $\Delta = 4 + 9\beta^2 + 4\gamma - 7\gamma^2 - 6\beta(2+\gamma)$. Hence all states $\rho_{\alpha,\beta,\gamma}$ with constraints (43) are either bound entangled our separable, whereas the others are NPT entangled.

From the realignment criterion we obtain the constraints

$$\alpha \leq \frac{1}{16}\left(6 + 11\beta - \gamma - \Delta_1\right) \tag{44}$$
$$\alpha \leq \frac{1}{16}\left(6 + 11\beta - \gamma + \Delta_1\right) \tag{45}$$
$$\alpha \geq \frac{1}{16}\left(-6 + 11\beta - \gamma - \Delta_2\right) \tag{46}$$
$$\alpha \geq \frac{1}{16}\left(-6 + 11\beta - \gamma + \Delta_2\right) \tag{47}$$

where

$$\begin{aligned} \Delta_1 &:= \sqrt{4 + 36\beta + 81\beta^2 - 12\gamma - 54\beta\gamma + 33\gamma^2} \quad \text{and} \\ \Delta_2 &:= \sqrt{4 - 36\beta + 81\beta^2 + 12\gamma - 54\beta\gamma + 33\gamma^2}. \end{aligned} \tag{48}$$

Only constraint (44) is violated by some PPT states, which thus have to be bound entangled. The PPT entangled states exposed by the realignment criterion are therefore concentrated in the region confined by the constraints

$$\alpha \leq \frac{7}{2}\beta + 1 - \gamma,\ \alpha \leq \frac{1}{16}\left(-2 + 11\beta + 3\sqrt{\Delta}\right),\ \alpha \geq \frac{1}{16}\left(6 + 11\beta - \gamma - \Delta_1\right). \tag{49}$$

The three-parameter family (39) also bears the advantage that it can be nicely illustrated by the Euclidean geometry. To do this, note that the orthogonality conditions of the Hilbert-Schmidt space $\mathcal{A}$ have to be transferred correctly, which is achieved by choosing a nonorthogonal and differently scaled coordinate system of parameter axes α, β, and γ. They are chosen such that they each become orthogonal to one of the boundary planes of the set of the three-parameter family of states, given by the positivity constraints (40). In order to calculate quantities well known in an Euclidean space spanned by an orthogonal equally scaled coordinate system, we have to transform points of the non-orthogonal coordinates (α, β, γ) into points of orthogonal coordinates (a, b, c) and vice versa by

$$a = \alpha - \frac{1}{8}\beta - \frac{1}{8}\gamma,\ b = \frac{\sqrt{3}}{8}\left(3\beta - \gamma\right),\ c = \frac{\sqrt{3}}{4}\gamma. \tag{50}$$

In Fig. 3 the three-parameter family of states $\rho_{\alpha,\beta,\gamma}$ (39) including NPT entangled, PPT entangled (bound entangled) and further PPT states are illustrated in the Euclidean geometry picture. In Refs. [38, 42] we applied the outside-in shift method to detect most of the bound entangled states (49), where a version of Lemma 1 (for Weyl operator decompositions) was used to show that for particular parameter regions geometric operators correspond to geometric entanglement witnesses. The geometric shifting operators G_λ (29) were constructed on lines between bound entangled starting states $\rho = \rho_b^{\mathrm{BE}}$ on the Horodecki line (41) and the maximally mixed state, $\tilde{\rho} = (1/9)\mathbb{1}$.

Actually all PPT entangled states of Eq. (49), Fig. 3, can be detected using Lemma 1. To see this, we construct tangent planes onto the surface of the function

$$\alpha = \frac{1}{16}\left(6 + 11\beta - \gamma - \Delta_1\right) \tag{51}$$

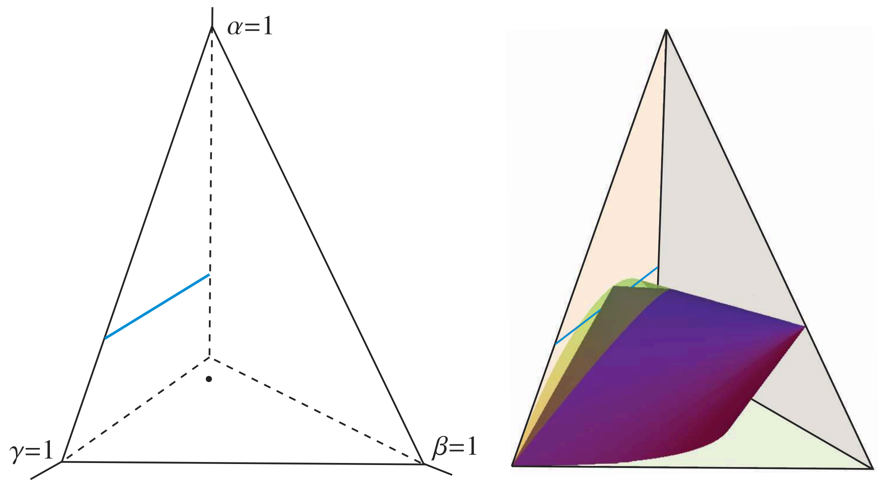

FIG. 3: Illustration in of the family of states $\rho_{\alpha,\beta,\gamma}$ (39) in the Euclidean geometry. Left: All states $\rho_{\alpha,\beta,\gamma}$ lie within a pyramid due to the positivity constraints (40). The dot represents the origin of the coordinate axes, which is the maximally mixed state $(1/9)\mathbb{1}$. The line (blue) on the left boundary plane represents the Horodecki states (41). Right: Illustration of the PPT and realignment criteria. The cone with tip on the right vertex line of the pyramid contains the PPT states, which is intersected by a cone (tip on the left boundary plane of the pyramid) of states that satisfy the realignment criterion, and hence PPT entangled states can be revealed (translucent yellow region). All other states of the pyramid are NPT entangled.

from the realignment criterion (44), where we use orthogonal coordinates (50). In this way we can assign geometric operators to the tangential plane by choosing points $\vec{a}$ inside the planes and points $\vec{b}$ outside the planes such that $\vec{a}-\vec{b}$ is orthogonal to the planes. Since the Euclidean geometry of our picture is isomorphic to the Hilbert-Schmidt geometry, the points $\vec{a}$ and $\vec{b}$ correspond to states ρ_a and ρ_b and we can construct the geometric operator accordingly,

$$G_{\mathrm{re}} = \rho_a - \rho_b - \langle \rho_a, \rho_a - \rho_b \rangle \mathbb{1}_9 \,. \tag{52}$$

This operators (52) are linear combinations of the three-parameter states $\rho_{\alpha,\beta,\gamma}$ which are linear combinations of the Bell states P_{nm} (34) and can be written as a Bloch decomposition using Eq. (38). First we need to define some expressions of Weyl operator combinations,

$$\begin{aligned} U_1 &:= U_{01}\otimes U_{01} + U_{02}\otimes U_{02} + U_{11}\otimes U_{-11} + U_{12}\otimes U_{-12} + U_{21}\otimes U_{-21} + U_{22}\otimes U_{-22}\,,\\ U_2 &:= U_2^I + U_2^{II} \qquad \text{with} \quad U_2^I := U_{10}\otimes U_{-10}\,, \quad U_2^{II} := U_{20}\otimes U_{-20}\,. \end{aligned} \tag{53}$$

The geometric operators (52) corresponding to tangent planes in points $(\alpha_{\mathrm{t}}, \beta_{\mathrm{t}}, \gamma_{\mathrm{t}})$, where α_{t} is a function of β_{t} and γ_{t}, given by the realignment function (51), are

$$\begin{aligned} G_{\mathrm{re}} &= a\,(2\,\mathbb{1} - U_1 + c\,U_2^I \, + \, c^* U_2^{II})\,, \quad \text{with} \\ a &= \frac{1}{36}\,(-2 - 9\beta_{\mathrm{t}} + 3\gamma_{\mathrm{t}} + 3\Delta_c)\,, \\ c &= \frac{9\gamma_{\mathrm{t}}^2 + (-2 - 9\beta_{\mathrm{t}} + 3\gamma_{\mathrm{t}})\Delta_c + \sqrt{3}\gamma_{\mathrm{t}}\,(2 + 9\beta_{\mathrm{t}} - 3\gamma_{\mathrm{t}} + 3\Delta_c)\,i}{(2+9\beta_{\mathrm{t}})^2 - 6(2+9\beta_{\mathrm{t}})\gamma_{\mathrm{t}} + 36\gamma_{\mathrm{t}}^2}\,, \\ \Delta_c &:= \sqrt{4 + 36 + 81\beta_{\mathrm{t}}^2 - 12\gamma_{\mathrm{t}} - 54\beta_{\mathrm{t}}\gamma_{\mathrm{t}} + 33\gamma_{\mathrm{t}}^2}\,. \end{aligned} \tag{54}$$

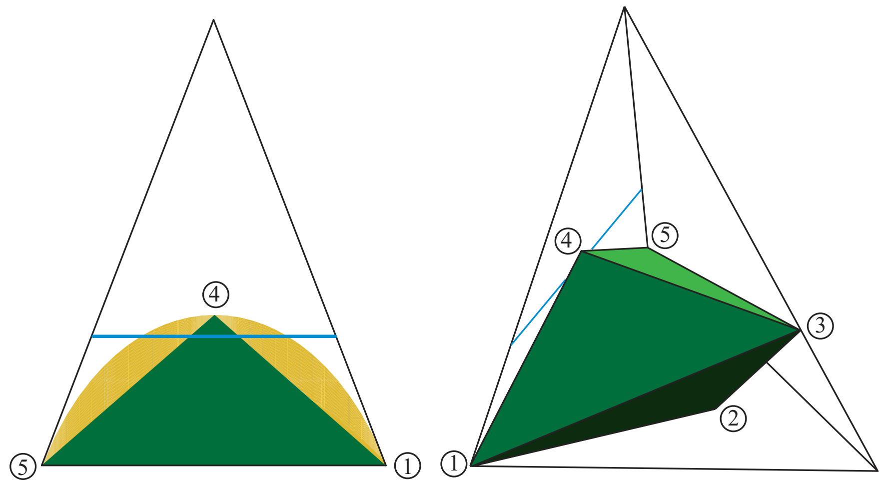

FIG. 4: Left: The entanglement properties of the three-parameter family on the boundary plane (56) where the Horodecki states are located. The triangular region (green) contains the separable states, the bound entangled states are located in the parabolic region (yellow), and the remaining states are NPT entangled. Right: The kernel polytope is a polygon (green) that includes states that are necessarily separable.

The singular values of the correlation coefficient matrix are the absolute values of the coefficients -1, c and c^* in Eq. (54), which are all one,

$$\{s_i\} = \{1,1,1,1,1,1,1,1\}\,, \tag{55}$$

and therefore, according to Lemma 1, the geometric operators $G_{\rm re}$ are entanglement witnesses that detect the entanglement of all states "above" the corresponding planes, thus also the bound entangled states in the region of Eq. (49).

We might ask ourselves if the PPT entanglement of Eq. (49), revealed by the realignment criterion and also by GEWs, is all there is for the three-parameter states (39). Or, to put it differently, are all the three-parameter states that satisfy *both* the PPT and the realignment criterion separable? We can answer this question by using GEWs and the inside-out shift method. The entanglement properties of the states on the boundary plane

$$\alpha = \frac{7}{2}\beta + 1 - \gamma \tag{56}$$

of the positivity pyramid are already fixed. The realignment function (51) and also the GEWs $G_{\rm re}$ (54) draw a triangle on this plane, whose vertices are separable states. The tip of the triangle is a separable state since it is PPT and $\gamma = 0$ (all PPT states of the two-parameter subset $\gamma = 0$ are separable, shown in Ref. [51]), the other two, at $\gamma = 1$ and $\gamma = -1$ are simple mixtures of Bell states P_{nm} that are also shown to be separable in Ref. [51]. So the the triangle is the convex hull of the three separable states and thus has to be separable. For an illustration of the entanglement properties on the boundary plane (56) see Fig. 4.

But what about all the three-parameter states (39)? First, we construct a kernel polytope of those states that are necessarily separable. This can be done by identifying five separable states that serve as vertices for the kernel polytope. Three arise from the two-parameter

subset $\gamma = 0$, where all PPT states are separable, the remaining two vertices are the separable states with $\gamma = 1$ and $\gamma = -1$ on the boundary plane (56). The resulting kernel polytope is a polygon with five vertices, see Fig. 4. Alternatively, one can also use sufficient criteria for separability to construct a kernel polytope of separable states. In Ref. [55] a sufficient separability criterion is presented that is shown to be applicable for states of the magic simplex.

In Ref. [43] it remained open if this polygon contains all separable states of the three-parameter family (39), which would imply much greater regions of bound entanglement than detected before. Here we want to show that this is not the case.

We can assign geometric operators to four boundary planes of the kernel polygon, in the same way as we did for the planes on the realignment surface, see Eq. (52), where we use the geometric isomorphism again. We call the four geometric operators $G^u_\pm, G^d_\pm$, which correspond to the following planes given by three vertex points (see Fig. 4): G^u_+ to $1, 3, 4$, G^u_- to $3, 4, 5$, G^d_+ to $1, 2, 3$, and G^d_- to $2, 3, 5$. The plus and minus sign indicates the side with positive or negative values of the parameter γ. The operators are

$$\begin{aligned} G^u_\pm &= a\,(2\,\mathbb{1} - U_1 + c\,U_2^I \,+\, c^* U_2^{II})\,, \quad \text{with } a = \frac{1}{63},\; c = -1 \pm \sqrt{3}i \\ G^d_\pm &= a\,(2\,\mathbb{1} + U_1 + c\,U_2^I \,+\, c^* U_2^{II})\,, \quad \text{with } a = \frac{1}{63},\; c = -1 \pm \sqrt{3}i \end{aligned} \tag{57}$$

The boundary planes can be easily shifted along parameterized lines through their normal vectors, and so can the assigned geometric operators (57). Note that we have a simplified picture of locally maximally mixed states, see Remark 3. The operators $G^u_\pm, G^d_\pm$ themselves are not entanglement witnesses, since the condition (24) can be numerically shown to be violated (see Corollary 2). The singular values are again the absolute values of the correlation coefficients, $\{s_i\} = \{1, 1, 1, 1, 1, 1, 2, 2\}$, hence Lemma 1 does not give an answer. It is difficult to show a violation analytically because of the complex Bloch vector geometry of qutrits, see Remarks 1 and 4. In order to check the condition (24) we minimize the left-hand term numerically by varying the possible Bloch vectors $\vec{n}^*, \vec{m}^*$, restricted by the condition $\rho \geq 0$ with ρ of Eq. (11). Shifting the operators outside, we find a minimum $S = -1$ of condition (24) when the planes become tangent to the shape enclosed by the PPT and realignment criterion, achieving new vertices at the touch points. Employing the inside-out shift method, see Sec. IV and Fig. 2, we construct a new polygon with the new vertices, and assign new geometric operators corresponding to the new boundary planes. Shifting the new operators outside, we again find the minimum $S = -1$ at planes tangent to the PPT and realignment shape. Therefore there is a very strong implication that the PPT and realignment shape, seen as the two-cone shape in Fig. 3, is the shape of the separable states. Fig. (3) thus is a picture of all entanglement properties of the three-parameter family.

VI. SUMMARY AND CONCLUSION

We use the concept of Bloch decompositions and entanglement witnesses to detect the entanglement properties of arbitrary dimensional bipartite quantum states. In particular we show how to reformulate the conditions of the entanglement witness criterion by using Bloch decompositions (Corollary 2) and formulated a sufficient condition for an operator to be an entanglement witness (Lemma 1).

We give the definition of a geometric operator and a geometric entanglement witness and explain two methods of "shifting" it (Proposition 1): One for the detection of bound entangled states, the *outside-in shift*, and one for the detection of separable states and for the construction of the shape of the set of separable states, the *inside-out shift*.

Finally we apply the previous results on a family of three-parameter two-qutrit states that are part of a simplex in the state space of two qutrits, the *magic simplex*. We show how to detect bound entangled states and construct the shape of separable states for this family. The results can be conveniently illustrated by the Euclidean geometry.

Our approach to entanglement detection is guided by the geometrically intuitive way of using entanglement witnesses. The construction of geometric entanglement witnesses directly uses the fact that entanglement witnesses correspond to hyperplanes in the Hilbert-Schmidt geometry. In this way it becomes easier to apply geometric operations like the shifting of planes. Using Bloch vector decompositions of operators and states we can furthermore simplify the conditions that have to be satisfied such that a geometric operator is a geometric entanglement witnesses. The construction of geometric entanglement witnesses does not rely on special properties of the states, i.e. it can be done for NPT or PPT entangled states likewise.

The presented example is relevant in many aspects. First of all the states of the magic simplex are a higher dimensional analogy of Bell-state mixtures of the two-qubit case that are relevant for quantum communication tasks, as explained in Sec. V. Furthermore it is interesting and surprising that this particular three-parameter family includes the Horodecki states that were among the first examples of bound entangled states. Thus the three-parameter family can be viewed as a more-parameter extension of the Horodecki states that includes even more bound entangled states. Finally the three-parameter states allow a nice Euclidean illustration that makes the regions of entangled, bound entangled and separable states visible.

Throughout the paper we restrict ourselves to bipartite states. Of course a multipartite extension is trivially possible if we only want to distinguish between states that contain entangled states in any of its particles and states that are fully separable into all particles. The definition of separable states just has to be extended with additional tensor products respectively. In the case of multipartite states one can distinguish between the distillability of states into entangled states of a fixed number of particles [56]. Entangled multipartite states can themselves be classified in different ways, for example with respect to the number of particles that are entangled. For details see, e.g., Refs. [57, 58, 59].

Acknowledgments

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